Ch 4.1 Numerical Differentiation

The derivative of a function f at x_0 is

$$f'(x_0) = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

$$= \lim_{h \to 0} \frac{f(x_0+h) - f(x_0)}{h}$$

$$\approx \frac{f(x_0+h) - f(x_0)}{h} \quad \text{(for small } h\text{)}$$

Not a good approximation, due to cancellation error, but a good place to start.

Suppose $x_0 \in (a,b)$ and $f \in C^2[a,b]$, with $x_1 = x_0 + h$ for $h \neq 0$ and $x_1 \in [a,b]$.

The Lagrange polynomial $P_{0,1}(x)$ interpolating f at x_0 and x_1 is used to approximate f:

$$f(x) = P_{0,1}(x) + \underbrace{\left[\frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x)) \right]}_{E(x)}$$

$$= \frac{(x-[x_0+h])}{x_0-[x_0+h]} f(x_0) + \frac{(x-x_0)}{(x_0+h)-x_0} f(x_0+h) + E(x)$$

$$= \frac{(x-x_0-h)}{-h} f(x_0) + \frac{(x-x_0)}{h} f(x_0+h) + \underbrace{\frac{(x-x_0)(x-x_0-h)}{2} f''(\xi(x))}_{E(x)}$$

We have

$$f(x) = \frac{(x-x_0-h)}{-h} f(x_0) + \frac{(x-x_0)}{h} f(x_0+h) + \overbrace{\frac{(x-x_0)(x-x_0-h)}{2} f''(\xi(x))}^{E(x)}$$

where $\xi(x) \in (a,b)$. Then

$$f'(x) = \frac{f(x_0)}{-h} + \frac{f(x_0+h)}{h} + \frac{d}{dx} E(x)$$

$$= \frac{f(x_0+h) - f(x_0)}{h} + \left[\frac{(x-x_0-h) + (x-x_0)}{2} \right] f''(\xi(x))$$

$$+ \frac{(x-x_0)(x-x_0-h)}{2} \cdot \frac{d}{dx} f''(\xi(x))$$

$$= \frac{f(x_0+h) - f(x_0)}{h} + \left[\frac{2(x-x_0) - h}{2} \right] f''(\xi(x))$$

$$+ \frac{(x-x_0)(x-x_0-h)}{2} f'''(\xi(x)) \cdot \xi'(x)$$

Since $\xi(x)$ is unknown, our error term is incomplete. However, for $x = x_0$ we have

$$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{h}{2} f''(\xi(x_0))$$

where $\xi(x_0) \in (a,b)$.

Thus $f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{h}{2} f''(\xi(x_0))$

our error term is thus bounded by

$$\frac{Mh}{2}, \text{ where } M = \max_{x \in [a,b]} |f''(x)| ,$$

when we use

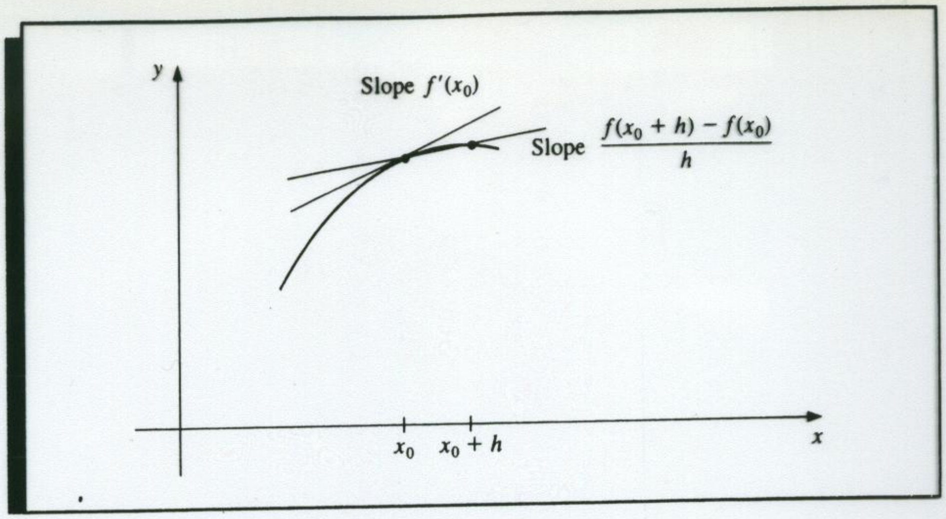
$$f'(x_0) \cong \frac{f(x_0+h) - f(x_0)}{h} . \quad (*)$$

When $h>0$, equation (*) is known as the forward difference formula.

When $h<0$, equation (*) is known as the backward difference formula.

See Example 1 in text.

Figure 4.1



EXAMPLE 1 Let $f(x) = \ln x$ and $x_0 = 1.8$. The forward-difference formula

$$\frac{f(1.8+h) - f(1.8)}{h}$$

is used to approximate $f'(1.8)$ with error

$$\frac{|hf''(\xi)|}{2} = \frac{|h|}{2\xi^2} \leq \frac{|h|}{2(1.8)^2}, \quad \text{where} \quad 1.8 < \xi < 1.8 + h.$$

The results in Table 4.1 are produced when $h = 0.1$, 0.01, and 0.001.

Table 4.1

h	$f(1.8+h)$	$\frac{f(1.8+h)-f(1.8)}{h}$	$\frac{\lvert h\rvert}{2(1.8)^2}$
0.1	0.64185389	0.5406722	0.0154321
0.01	0.59332685	0.5540180	0.0015432
0.001	0.58834207	0.5554013	0.0001543

Since $f'(x) = 1/x$, the exact value of $f'(1.8)$ is $0.55\overline{5}$, and the error bounds are quite close to the true approximation error. ∎

Math 361 Numerical Analysis — Ch 4.1 Numerical Differentiation

Using Excel

Problem 1b					Problem 3b		
		f'(x)					
x	f(x)	forward diff	back diff	f'(x(k))	fwd diff error	bwd diff error	Error Bound
0.0	0.00000						
0.2	0.74140						
0.4	1.37180						
f(x) = exp(x) -2x^2+3x-1							
f '(x) = exp(x) - 4x + 3							
f "(x) = exp(x) - 4							
Error Bound = | Max f "(x)*h/2 |			(Show your calculations here)				

Three Point Formula

Suppose $\{x_0, x_1, x_2\}$ are distinct numbers in $[a,b]$ and $f \in C^3[a,b]$. We have

$$f(x) = \sum_{k=0}^{2} f(x_k) L_{2,k}(x) + \frac{(x-x_0)(x-x_1)(x-x_2)}{3!} f'''(\xi(x))$$

where $\xi(x) \in [a,b]$. Then

$$f'(x) = \sum_{k=0}^{2} f(x_k) L'_{2,k}(x) + \left[\frac{d}{dx}\frac{(x-x_0)(x-x_1)(x-x_2)}{6}\right] f'''(\xi(x))$$

$$+ \frac{(x-x_0)(x-x_1)(x-x_2)}{6} \cdot \frac{d}{dx} f'''(\xi(x))$$

If $x = x_j$, for $j \in \{0,1,2\}$, then

$$f'(x_j) = \sum_{k=0}^{2} f(x_k) L'_{2,k}(x_j) + \left[\prod_{\substack{k=0 \\ k \neq j}}^{2} (x_j - x_k)\right] \frac{f'''(\xi(x_j))}{6}$$

Now

$$L_{2,0}(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} \Rightarrow L'_{2,0}(x) = \frac{2x - x_1 - x_2}{(x_0-x_1)(x_0-x_2)}$$

$$L'_{2,1}(x) = \frac{2x - x_0 - x_2}{(x_1-x_0)(x_1-x_2)}, \quad L'_{2,2}(x) = \frac{2x - x_0 - x_1}{(x_2-x_0)(x_2-x_1)}$$

(Show)

We have, for $j = 0, 1, 2$,

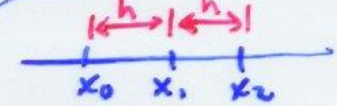
$$f'(x_j) = f(x_0)\left[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}\right]$$

$$+ f(x_1)\left[\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}\right]$$

$$+ f(x_2)\left[\frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}\right]$$

$$+ \frac{1}{6} f'''(\xi(x_j)) \prod_{\substack{k=0 \\ k \neq j}}^{2} (x_j - x_k),$$

where $\xi(x_j) \in (a, b)$.



Suppose nodes equally spaced by h:

$$x_0, \quad x_1 = x_0 + h, \quad x_2 = x_0 + 2h$$

Then

$$f'(x_0) = f(x_0)\left[\frac{2x_0 - x_1 - x_2}{(-h)(-2h)}\right] + f(x_1)\left[\frac{2x_0 - x_0 - x_2}{(h)(-h)}\right]$$

$$+ f(x_2)\left[\frac{2x_0 - x_0 - x_1}{(2h)(h)}\right] + \frac{1}{6} f'''(\xi(x_0))(x_0 - x_1)(x_0 - x_2)$$

$$= f(x_0) \cdot \left(-\frac{3}{2h}\right) + f(x_1)\left(\frac{2}{h}\right) + f(x_2)\left(-\frac{1}{2h}\right)$$

$$+ \frac{1}{6} f'''(\xi(x_0)) \cdot (-h)(-2h)$$

Thus

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_1) - \frac{1}{2}f(x_2)\right] + \frac{h^2}{3}f'''(\xi(x_0))$$

Similarly,

$$f'(x_1) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_2)\right] - \frac{h^2}{6}f'''(\xi(x_1))$$

$$f'(x_2) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_1) + \frac{3}{2}f(x_2)\right] + \frac{h^2}{3}f'''(\xi(x_2))$$

Since $x_1 = x_0 + h$, and $x_2 = x_0 + 2h$, we have

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_0+h) - \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{3}f'''(\xi(x_0))$$

$$f'(x_0+h) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_0+2h)\right] - \frac{h^2}{6}f'''(\xi(x_1))$$

$$f'(x_0+2h) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_0+h) + \frac{3}{2}f(x_0+2h)\right] + \frac{h^2}{3}f'''(\xi(x_2))$$

In 2^{nd} & 3^{rd} formulas, replace x_0+h and x_0+2h by x_0, respectively:

$$f'(x_0) = \frac{1}{h}\left[-\frac{1}{2}f(x_0-h) + \frac{1}{2}f(x_0)\right] - \frac{h^2}{6}f'''(\xi(x_1))$$

$$f'(x_0) = \frac{1}{h}\left[\frac{1}{2}f(x_0-2h) \cancel{-2f(x_0)+\frac{3}{}} \rightarrow -2f(x_0-h) + \frac{3}{2}f(x_0)\right] + \frac{h^2}{3}f'''(\xi(x_2))$$

We have

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3} f'''(\xi(x_0))$$

$$f'(x_0) = \frac{1}{2h}\left[-f(x_0-h) + f(x_0+h)\right] - \frac{h^2}{6} f'''(\xi(x_1))$$

$$f'(x_0) = \frac{1}{2h}\left[f(x_0-2h) - 4f(x_0-h) + 3f(x_0)\right] + \frac{h^2}{3} f'''(\xi(x_2))$$

Note that the 3rd equation can be obtained from the 1st by replacing h by $-h$. That means we will focus only on the first two formulas: (Both are considered 3 pt formulas)

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \underline{\frac{h^2}{3} f'''(\xi(x_0))}$$

$$f'(x_0) = \frac{1}{2h}\left[-f(x_0-h) + f(x_0+h)\right] - \underline{\frac{h^2}{6} f'''(\xi(x_1))}$$

We may assume that

$$\xi(x_0) \in (x_0, x_0+2h), \quad \xi(x_1) \in (x_0-h, x_0+h)$$

- Both formulas for $f'(x_0)$ have error of $O(h^2)$, athough the 2nd error is about half the first.
- The 1st formula requires 3 evaluations of f, all to right of x_0; 2nd formula just 2, on each side of x_0.

$$f'(x_1) = f(x_0)\left[\frac{2x_1 - x_1 - x_2}{(x_0-x_1)(x_0-x_2)}\right]$$

$$+ f(x_1)\left[\frac{2x_1 - x_0 - x_2}{(x_1-x_0)(x_1-x_2)}\right]$$

$$+ f(x_2)\left[\frac{2x_1 - x_0 - x_1}{(x_2-x_0)(x_2-x_1)}\right]$$

$$+ \frac{1}{6} f'''(\xi(x_1)) \prod_{\substack{k=0 \\ k\neq 1}}^{2} (x_1 - x_k)$$

$$= f(x_0)\left[\frac{x_1 - x_2}{(x_0-x_1)(x_0-x_2)}\right] + f(x_1)\left[\frac{2x_1 - x_0 - x_2}{(x_1-x_0)(x_1-x_2)}\right]$$

$$+ f(x_2)\left[\frac{x_1 - x_0}{(x_2-x_0)(x_2-x_1)}\right] + \frac{1}{6} f'''(\xi(x_1))(x_1 - x_0)(x_1-x_2)$$

$\begin{pmatrix} x_1 = x_0 + h \\ x_2 = x_0 + 2h \end{pmatrix}$

$$= f(x_0)\left[\frac{-h}{(-h)(-2h)}\right] + f(x_1)\left[\frac{0}{(h)(-h)}\right] + f(x_2)\left[\frac{h}{(2h)(h)}\right]$$

$$+ \frac{1}{6} f'''(\xi(x_1))(h)(-h)$$

$$= f(x_0)\left(-\frac{1}{2h}\right) + f(x_2)\left(\frac{1}{2h}\right) - \frac{h^2}{6} f'''(\xi(x_1))$$

$$= \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_2)\right] - \frac{h^2}{6} f'''(\xi(x_1))$$

Example 2

$\leftarrow f(x) = xe^x$

Values for $\boxed{f(x) = xe^x}$ are given in Table 4.2.

Table 4.2

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)] + \frac{h^2}{3}f'''(\xi_0)$

$f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6}f'''(\xi_1)$

Since $f'(x) = (x+1)e^x$, we have $f'(2.0) = 22.167168$. Approximating $\boxed{f'(2.0)}$ using the various three- and five-point formulas produces the following results.

Three-Point Formulas

Using (4.4) with $h = 0.1$: $\frac{1}{0.2}[-3f(2.0) + 4f(2.1) - f(2.2)] = 22.032310$,

Using (4.4) with $h = -0.1$: $\frac{1}{-0.2}[-3f(2.0) + 4f(1.9) - f(1.8)] = 22.054525$,

Using (4.5) with $h = 0.1$: $\frac{1}{0.2}[f(2.1) - f(1.9)] = 22.228790$,

Using (4.5) with $h = 0.2$: $\frac{1}{0.4}[f(2.2) - f(1.8)] = 22.414163$.

The errors in the formulas are approximately

$$1.35 \times 10^{-1}, \quad 1.13 \times 10^{-1}, \quad -6.16 \times 10^{-2}, \quad \text{and} \quad -2.47 \times 10^{-1},$$

respectively. (Here, actual error was computed : $|p - p^*|$)

Five-Point Formula

Using (4.6) with $h = 0.1$ (the only five-point formula applicable):

$$\frac{1}{1.2}[f(1.8) - 8f(1.9) + 8f(2.1) - f(2.2)] = 22.166999.$$

The error in this formula is approximately

$$1.69 \times 10^{-4}.$$

The five-point formula is clearly superior. Note also that the error from Eq. (4.5) with $h = 0.1$ is approximately half of the magnitude of the error produced using Eq. (4.4) with either $h = 0.1$ or $h = -0.1$. ■

See Excel sheet for more examples.

Problem 5b					Problem 7b		
		f'(x)					
x	f(x)	Eqn 4.4	Eqn 4.5	f'(x)	Eqn 4.4 Error	Eqn 4.5 Error	Error Bound
8.1	16.94410						
8.3	17.56492						
8.5	18.19056						
8.7	18.82091						

f(x) = x ln(x)
f '(x) = ln(x) + 1
f ''(x) = 1/x
f '''(x) = -1/x^2

Eqn 4.4 Error Bound = | Max f '''(x)*(h^2)/3 | (Show your calculations)

Eqn 4.5 Error Bound = | Max f '''(x)*(h^2)/6 | (Show your calculations)

Analysis of Roundoff Error

Consider the three-point formula

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6} f'''(\xi(x_0))$$

Suppose that, due to roundoff error, our computed values in this formula are

$$f(x_0+h) = \tilde{f}(x_0+h) + e(x_0+h)$$

$$f(x_0-h) = \tilde{f}(x_0-h) + e(x_0-h)$$

Then the total error in approximating $f'(x_0)$ is

$$f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h}$$

$$= \underbrace{\frac{e(x_0+h) - e(x_0-h)}{2h}}_{\text{roundoff error}} - \underbrace{\frac{h^2}{6} f'''(\xi(x_1))}_{\text{truncation error of interp polyn.}}$$

Suppose $|e(x_0 \pm h)| < \varepsilon$, for some $\varepsilon > 0$, and $|f'''(x)| \le M$, for $x \in [a,b]$. Then

$$\left| f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} \right| \le \frac{\varepsilon}{h} + \frac{h^2}{6} M$$

(Show.) <u>Note</u>: As $h \to 0$, roundoff error gets bigger.

Justification of Error Bound on Previous Slide

Recall

$$\left| f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} \right| = \left| \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f'''(\xi(x_1)) \right|$$

$$\le \frac{|e(x_0+h)|}{2h} + \frac{|e(x_0-h)|}{2h} + \frac{h^2}{6} |f'''(\xi(x_1))|$$

$$\le \frac{\varepsilon}{2h} + \frac{\varepsilon}{2h} + \frac{h^2}{6} M$$

$$= \frac{\varepsilon}{h} + \frac{h^2}{6} M,$$

where $M = \max_{x \in [a,b]} |f'''(x)|$.

Since roundoff error ε/h increases as h decreases, we typically cannot use h for very small values. (That is, use an h that is small but not too small.)

Example $f(x) = \sin x$; approximate $f'(0.9)$.
Note: True value is $f'(0.9) = \cos(0.9) = 0.62191$
See Tables in text. Here,

$$f'(0.900) \cong \frac{f(0.900+h) - f'(0.900-h)}{2h}$$

Recall that the error is bounded by:

$$|Error| \leq E(h) = \frac{\varepsilon}{h} + \frac{h^2}{6} M$$

To find min $E(h)$, take derivative:

$$E'(h) = -\frac{\varepsilon}{h^2} + \frac{h}{3} M \overset{set}{=} 0$$

$$\Rightarrow \frac{h}{3} M = \frac{\varepsilon}{h^2}$$

$$\Rightarrow h^3 = 3\varepsilon / M$$

$$\Rightarrow h = \sqrt[3]{3\varepsilon/M},$$

where $M = \max_{x\in[0.8,1.0]} |f'''(x)| = \max_{x\in[0.8,1.0]} |\cos(x)|$

$$= \cos(0.8) \cong 0.69671$$

An estimate for ε is $\varepsilon = 0.000005$, since the values of f in tables are given to five decimal places. Thus choose $h \cong 0.028$.

Table 4.3

x	$\sin x$	x	$\sin x$
0.800	0.71736	0.901	0.78395
0.850	0.75128	0.902	0.78457
0.880	0.77074	0.905	0.78643
0.890	0.77707	0.910	0.78950
0.895	0.78021	0.920	0.79560
0.898	0.78208	0.950	0.81342
0.899	0.78270	1.000	0.84147

Table 4.4

h	Approximation to $f'(0.900)$	Error
0.001	0.62500	0.00339
0.002	0.62250	0.00089
0.005	0.62200	0.00039
0.010	0.62150	−0.00011
0.020	0.62150	−0.00011
0.050	0.62140	−0.00021
0.100	0.62055	−0.00106

Recall that the three-point formula

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6} f'''(\xi(x_0))$$

is used to approximate $f'(x_0)$:

$$f'(x_0) \cong \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right]$$

with total error

$$E(h) = \frac{\varepsilon}{h} + \frac{h^2}{6} M, \quad M = \max_{x \in [a,b]} |f'''(x)|$$

This illustrates the fact that numerical differentiation is unstable, since small values of h needed to reduce truncation error also cause the roundoff error to grow.

Math 361 Numerical Analysis **Ch 4.1 Numerical Differentiation**

Using Excel

Problem 1b					Problem 3b		
		f'(x)					
x	f(x)	forward diff	back diff	f'(x(k))	fwd diff error	bwd diff error	Error Bound
0.0	0.00000						
0.2	0.74140						
0.4	1.37180						
f(x) = exp(x) -2x^2+3x-1							
f '(x) = exp(x) - 4x + 3							
f "(x) = exp(x) - 4							
Error Bound = | Max f "(x)*h/2 |			(Show your calculations here)				

Problem 5b					Problem 7b		
		f'(x)					
x	f(x)	Eqn 4.4	Eqn 4.5	f'(x)	Eqn 4.4 Error	Eqn 4.5 Error	Error Bound
8.1	16.94410						
8.3	17.56492						
8.5	18.19056						
8.7	18.82091						
f(x) = x ln(x)							
f '(x) = ln(x) + 1							
f "(x) = 1/x							
f '"(x) = -1/x^2							
Eqn 4.4 Error Bound = | Max f '"(x)*(h^2)/3 |				(Show your calculations)			
Eqn 4.5 Error Bound = | Max f '"(x)*(h^2)/6 |				(Show your calculations)			

Ch 4.1 Examples

		f'(x)						
x	**f(x)**	**forward diff**	**back diff**	**f'(x(k))**	**fwd diff error**	**bwd diff error**	**fwd error bound**	**bwd error bound**
0.0	0.00000	3.70700		4.00000	0.29300		0.30000	
0.2	0.74140	3.15200	3.70700	3.42140	0.26940	0.28560	0.27786	0.30000
0.4	1.37180		3.15200	2.89182		0.26018		0.27786

f(x) = exp(x) -2x^2+3x-1
f '(x) = exp(x) - 4x + 3
f ''(x) = exp(x) - 4 < 0 on [0, 0.4]
f '''(x) = exp(x) > 0 on [0,0.4]

Error Bound = | Max f ''(x)*h/2 | (Show your calculations here)

		f'(x)						
x	**f(x)**	**Eqn 4.4**	**Eqn 4.5**	**f'(x)**	**Eqn 4.4 Error**	**Eqn 4.5 Error**	**Eqn 4.4 Error bound**	**Eqn 4.5 Error bound**
8.1	16.94410	3.09205		3.09186	0.00019		0.00020322	
8.3	17.56492	3.11643	3.11615	3.11626	0.00017	0.00011	0.00019355	0.00010161
8.5	18.19056	3.14025	3.13998	3.14007	0.00018	0.00009	0.00020322	0.00009677
8.7	18.82091	3.16353		3.16332	0.00020		0.00019355	

f(x) = x ln(x)
f '(x) = ln(x) + 1
f ''(x) = 1/x
f '''(x) = -1/x^2 < 0 on [8.1,8.7]
f ''''(x) = 2/x^3 > 0 on [8.1,8.7]

Eqn 4.4 Error Bound = | Max f '''(x)*(h^2)/3 | (Show your calculations)

Eqn 4.5 Error Bound = | Max f '''(x)*(h^2)/6 | (Show your calculations)